Novel software implementation of the T-matrix method for arbitrary con…gurations of single and clusters of composite nonspherical particles

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Abstract

In this paper we describe a T-matrix computer program for solving a large class of boundary-value problems in electromagnetic scattering theory. The code enables to investigate the case of one homogeneous and inhomogeneous (multilayered, composite) scatterer and the case of an arbitrary number of scatterers.

1 Introduction

One of the fastest and most powerful numerical tools for computing nonspherical light scattering using localized vector spherical functions is the T-matrix method [1]. The T-matrix is independent of the incident and scattered …elds and depends only on the shape, size parameter, and refractive index of the scattering particle as well as on its orientation with respect to the coordinate system. However, for particles with extreme geometries or particles with appreciable concavities the single spherical coordinate based null …eld method fails to converge. A number of modi…cations to the conventional null …eld method have been suggested to improve the numerical stability. One of these formal modi…cations is the null …eld method with discrete sources [2-3]. Essentially, this method entails the use of a number of elementary sources for approximating the surface current densities. The discrete sources are placed on a certain support in an additional region with respect to the region where the solution is required. Unknown discrete sources amplitudes which produces the surface densities are computed by using the null …eld condition of the total electric …eld inside the particle surface.

The T-matrix formalism with discrete sources can be extended in a simple manner for composite and multilayered particles. In this context, the earlier results on the T-matrix method concerning the scattering of an arbitrarily shaped particle with a nonconcentric, arbitrarily shaped inclusion or the scattering by an arbitrary number of scatterers, can be combined with these new results to apply to more general types of scattering problems.

2 Computation of the T-matrix

2.1 Homogeneous scatterer

The T-matrix formalism for a homogeneous scatterer has been presented in [3]. For solving the transmission boundary-value problem in the framework of the null-…eld method with discrete sources the scattering object is replaced by a set of surface current densities e and h, so that in the exterior domain the sources and …elds are exactly the same as those existing in the original scattering problem. A set of integral equations for the surface current densities e and h is derived for a variety of discrete sources. Physically, the set of integral equations in question guarantees the null-…eld condition inside the particle. It is noted that localized and distributed vector spherical

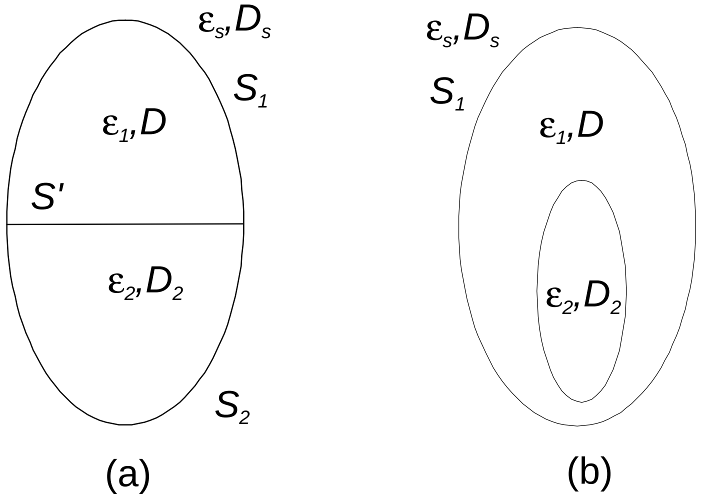

Figure 1: Geometry of the scattering problem: (a)-composite scatterer, and (b)-multilayered scatterer.

functions, magnetic and electric dipoles or vector Mie-potentials can be used as discrete sources. The surface current densities are then approximated by fields of discrete sources corresponding to the internal problem. Once the surface current densities are determined the scattered field outside the circumscribing sphere is obtained by using the representation theorem. Finally, the transition matrix is obtained by assuming spherical vector wave expansions for the incident and the scattered field.

2.2 Composite scatterer

For the generic case of a composite scatterer that consists of two homogeneous parts (see Figure 1a) we use the Stratton-Chu representation theorem to write the general null-field equations in the form

$$E_0(x) + \sum_{i=1}^{2} \nabla \times \int_{S_i \cup S'} e_i(y) g_s(x,y)\, dS + \frac{j}{k_0 \varepsilon_s} \nabla \times \nabla \times \int_{S_i \cup S'} h_i(y) g_s(x,y)\, dS = 0; \qquad (1)$$

where $x \in D_i;\ i = 1, 2$. An infinite set of equations for the surface current densities is derived by imposing the null-field conditions separately in each domain D_i. The infinite set of integral equations may be formulated in terms of localized and distributed spherical vector wave functions. The surface current densities e_i, h_i, $i = 1, 2$, are approximated by linear combinations of discrete sources satisfying the Maxwell's equations in each interior domain. The transition matrix is then obtained by using the representation theorem for the scattered field.

2.3 Multilayered scatterer

The generic situation consisting in a two-layered scatterer defined by the closed surfaces S_1 and S_2, where S_1 encloses S_2, is depicted in Figure 1b. The general null-field conditions are

$$E_0(x) + \nabla \times \int_{S_1} e_1(y) g_s(x,y)\, dS + \frac{j}{k_0 \varepsilon_s} \nabla \times \nabla \times \int_{S_1} h_1(y) g_s(x,y)\, dS = 0; \qquad (2)$$

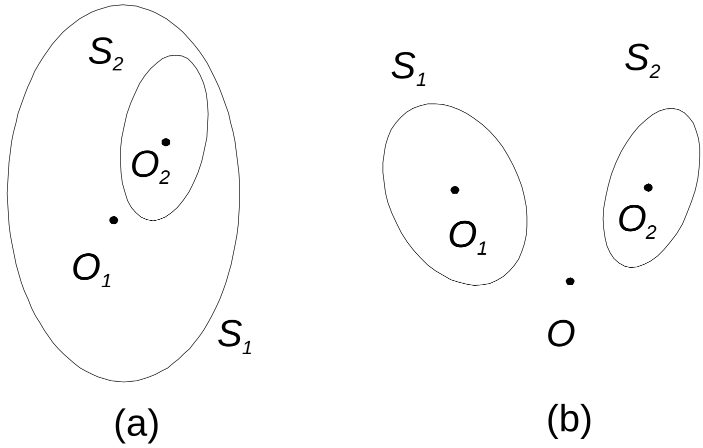

Figure 2: Geometry of the scattering problem: (a)-scatterer with a nonspherical inclusion, and (b)-systems of scatterers.

for $x \in D_1$; and

$$\sum_{i=1}^{2} (-1)^i \left[\nabla \times \int_{S_i} e_i(\cdot) g_1(x,\cdot) dS + \frac{j}{k_0 \varepsilon_1} \nabla \times \nabla \times \int_{S_i} h_i(\cdot) g_1(x,\cdot) dS \right] = 0, \quad (3)$$

for $x \in D_s$ and $x \in D_2$. The above general null-field equations may be converted into a set of integral equations for the surface densities in the variety of discrete sources. For computing the transition matrix we approximate the surface densities e_1 and h_1 acting on S_1 by fields of regular and radiating discrete sources, while the surface densities e_2 and h_2 acting on S_2 are approximated by fields of regular sources.

2.4 Scatterers with nonspherical inclusions and systems of scatterers

By invoking the results of the preceding sections and relying on the formulations of References [4-5] we may compute the total transition matrices for some complex structures. The transition matrix of a scatterer containing a nonspherical inclusion as shown in Figure 2a is given by

$$T_{12} = T_1 - Q_1^{1,3} \hat{T}_2 \left(Q_1^{3,1}\right)^{-1} \left[I - Q_1^{3,3} \hat{T}_2 \left(Q_1^{3,1}\right)^{-1} \right]^{-1}, \quad (4)$$

where $\hat{T}_2 = \sigma^1_{O_1O_2} T_2 \sigma^1_{O_2O_1}$. Here, T_1 and T_2 are the transition matrix of the host particle and of the inclusion, $\sigma^1_{OO_1}$ is the rototranslation matrix passing from the origin O to the origin O_1, and $Q_1^{i,j}$ have the same significance as in [5].

For a system of two particles as pictured in Figure 2b we have

$$\begin{aligned} T_{12} = {} & \sigma^1_{OO_1} T_1 \left[I - \sigma^3_{O_1O_2} T_2 \sigma^3_{O_2O_1} T_1 \right]^{-1} \left[\sigma^3_{O_1O_2} T_2 \sigma^1_{O_2O} + \sigma^1_{O_1O} \right] \\ & + \sigma^1_{OO_2} T_2 \left[I - \sigma^3_{O_2O_1} T_1 \sigma^3_{O_1O_2} T_2 \right]^{-1} \left[\sigma^3_{O_2O_1} T_1 \sigma^1_{O_1O} + \sigma^1_{O_2O} \right]; \end{aligned} \quad (5)$$

where T_1 and T_2 stands for the transition matrices of the scatterers bounded by the surfaces S_1 and S_2; respectively.

The above results may simply be combined to obtain the total T-matrix for new classes of scattering con…gurations, as for example the case of several multilayered scatterers or the case of one scatterer which contains several inclusions.

3 Conclusion

An e¢cient way for computing the transition matrix in the framework of the null-…eld method with discrete sources is presented. The extension of the formalism from the case of homogeneous scatterer to the case of composite and multilayered scatterer improves the performances of the T-matrix method for electromagnetic calculations.

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